Accurate Estimates of the Generalization Ability for Symmetric Set of Predictors and Randomized Learning Algorithms

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Abstract—The main issue of the combinatorial approach to overfitting is to obtain computationally efficient formulas for overfitting probabilities. A group-theoretical approach is proposed to simplify derivation of such formulas when the set of predictors has a certain group of symmetries. Examples of the sets are given. The general estimate of overfitting probability is proved for the randomized learning algorithm. It is applied to four model sets of predictors—a layer of the Boolean cube, the Boolean cube, the unimodal chain, and a bundle of monotonic chains.

Key words: statistical learning theory, generalizing ability, overfitting probability, empirical risk minimization (ERM), randomized learning algorithm, group of symmetries, group orbit, monotonic chain of predictors, bundle of monotonic chains.

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1. INTRODUCTION

The problem of choice under incomplete information always accompanies pattern recognition, regression restoration, and forecasting problems. Given only a finite learning sample of objects, one needs to choose the predictor from the given set of predictors that would make as few errors as possible on the objects from both the observable learning sample and the hidden test sample not known when the predictor is chosen. If the frequency of errors of the test sample exceeds that of the learning sample, we speak of overfitting of the predictor, i.e., being too good in describing particular data, it cannot generalize it, restore the pattern that generated it, or be used to make predictions.

The frequency of errors on the learning sample is also called *empirical risk*. *Empirical risk minimization* (ERM) is the learning algorithms that chooses such predictor from the given set, that makes the fewest number of errors on the learning sample [1, 2]. The table gives an example of empirical risk minimization leading to overfitting. The columns of the table stand for the predictors; its rows, for the objects of the learning sample $\{x_1, x_2, x_3\}$ and the test sample $\{x_4, x_5, x_6\}$. The unity in the $[i, d]$-th cell of the table means that the predictor a_d makes an error on the object x_i.

	a_1	a_2	…	a_d	…	a_d
x_1	0	1	…	0	…	1
x_2	1	1	…	0	…	0
x_3	0	0	…	0	…	0
x_4	1	1	…	1	…	1
x_5	1	0	…	1	…	0
x_6	0	0	…	1	…	0

In this example, overfitting may result from a "bad" decomposition of the general sample into learning and test samples. Therefore, we introduce the functional of *overfitting probability* that equals the part of decompositions of the sample that cause overfitting [3, 4]. This functional is invariant to the choice of the decomposition and characterizes the quality of the learning algorithm for the given general sample.

For some families of simple structure (monotonic and unimodal chains and h-dimensional grids), accurate expressions of the overfitting probability are found in [3, 5]. In this work, we develop the group-theoretical approach [6] that helps estimate the overfitting probability efficiently for sets of predictors possessing symmetry properties.

1.1. Definitions

Let the general sample $\mathbb{X} = (x_1, ..., x_L)$ consisting of L objects be given. An arbitrary classification predictor applied to this sample generates a binary vector of

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errors $a \equiv (a(x_i))_{i=1}^{L}$, where $a(x_i) = 1$ means that the predictor a makes an error on the object x_i. We assume the general sample $\mathbb{X}$ to be fixed; therefore, the predictors are identified with their vectors of errors.

We use $\mathbb{A} = \{0, 1\}^L$ to denote the set of all possible vectors of errors of length L. Then, $2^{\mathbb{A}}$ is the set of all subsets of $\mathbb{A}$. Note that $|\mathbb{A}| = 2^L$, $|2^{\mathbb{A}}| = 2^{2^L}$.

We use $[\mathbb{X}]^l$ to denote the set of all decompositions of the general sample $\mathbb{X}$ into the learning sample X of length l and the test sample $\bar{X}$ of length $k = L - l$.

We denote *the number of errors* of the predictor a on the sample $U \subseteq \mathbb{X}$ by $n(a, U) = \sum_{x \in U} a(x)$.

An arbitrary mapping of the form $\mu: 2^{\mathbb{A}} \times [\mathbb{X}]^l \longrightarrow \mathbb{A}$ is called *the deterministic learning algorithm*. The learning algorithm μ uses the learning sample X to choose some predictor $a = \mu(A, X)$ from the subset $A \subseteq \mathbb{A}$. The learning algorithm is called *empirical risk minimization* if the predictor it returns makes a minimal number of errors in the course of training; i.e., for all $X \in [\mathbb{X}]^l$ and $A \subseteq \mathbb{A}$ $\mu(A, X) \in A(X)$ holds, where

$$A(X) = \operatorname*{Argmin}_{a \in A} n(a, X).$$

Empirical risk minimization can be ambiguous; i.e., several predictors from $A(X)$ can have the same number of errors on the learning sample. In [4], *pessimistic* empirical risk minimization was used to eliminate ambiguity and obtain accurate upper estimates of the overfitting probability, assuming that the predictor with the maximal number of errors on the general sample $\mathbb{X}$ is chosen in the case of ambiguity. This does not eliminate ambiguity for good. There can be cases when several predictors have a minimal number of errors on the learning sample X and the same number of errors on the general sample $\mathbb{X}$. In such cases, the set of predictors had a linear order introduced for it, with the predictor with a greater order number chosen among indistinguishable predictors. Setting priorities for the predictors is artificial, with no proper analogues among known learning algorithms.

1.2. Randomized Learning Algorithm

A randomized learning algorithm matches an arbitrary set of predictors $A \subseteq \mathbb{A}$ and an arbitrary learning sample $X \in [\mathbb{X}]^l$ with the weight distribution function on the set of predictors

$$\mu: 2^{\mathbb{A}} \times [\mathbb{X}]^l \longrightarrow \{f: \mathbb{A} \longrightarrow [0, 1]\}. \quad (1)$$

Naturally, we can assume this function to be normalized and interpreted as the probability to obtain each predictor as a result of training.

The deterministic learning algorithm is a special case of the randomized method when the weight distribution function $f(a)$ takes the unity value exactly on one predictor and the zero value on all other predictors.

Note that there is an equivalent way to give the mapping from definition (1)

$$\mu: 2^{\mathbb{A}} \times [\mathbb{X}]^l \times \mathbb{A} \longrightarrow [0, 1].$$

Let S_L be a permutation group, consisting of $L!$ elements. This group acts on the set of objects of the general sample by all possible permutations $\pi: \mathbb{X} \longrightarrow \mathbb{X}$.

For each $\pi \in S_L$, we give the way π acts upon the arbitrary sample $X \in [\mathbb{X}]^l$ as a mapping $\pi: \mathbb{X} \longrightarrow \mathbb{X}$ that acts upon each object of the sample X: $\pi X = \{\pi x: x \in X\}$ on an element-wise basis. The mapping does not change the number of objects $|X| = |\pi X|$, so we can speak about π acting on the set of decompositions of the general sample into training and test samples of the fixed length $\pi: [\mathbb{X}]^l \longrightarrow [\mathbb{X}]^l$.

We assume that, applied to the set of all predictors $\mathbb{A}$, S_L permutates vectors of errors of predictors $(\pi a)(x_i) = a(\pi^{-1}x_i)$. Here, objects are subjected to the inverse permutation π^{-1} since it is in this case when it is correct to say that the group S_L *acts* on the set $\mathbb{A}$.

Lemma 1.1. The number of errors of the predictor a on the subsample $U \subseteq \mathbb{X}$ remains the same after the permutation $\pi \in S_L$ is simultaneously applied to the predictor and the subsample

$$n(a, U) = n(\pi a, \pi U). \quad (2)$$

Proof. We write the definition of the number of errors of the predictor and use the action of the permutation π on the predictor a defined above

$$n(\pi a, \pi U) = \sum_{x_i \in \pi U} (\pi a)(x_i) = \sum_{x_i' \in U} (\pi a)(\pi x_i')$$

$$= \sum_{x_i' \in U} a(\pi^{-1}(\pi x_i')) = \sum_{x_i' \in U} a(x_i') = n(a, U).$$

The action of the group S_L on the set of all possible predictors $\mathbb{A}$ is naturally extended to the system of all subsets $S_L: 2^{\mathbb{A}} \longrightarrow 2^{\mathbb{A}}$ by the rule $\pi A = \{\pi a: a \in A\}$. In what follows, we use the single designation π for the actions described above.

Now, we can give a stricter definition of a randomized learning algorithm.

Definition 1. We call a *randomized learning algorithm* the mapping of the form

$$\mu: 2^{\mathbb{A}} \times [\mathbb{X}]^l \times \mathbb{A} \longrightarrow [0, 1] \quad (3)$$

that satisfies the following conditions for any $A \in 2^{\mathbb{A}}$, $X \in [\mathbb{X}]^l$, $a, b \in A$ and $\pi \in S_L$

(1) normalization

$$\sum_{a \in A} \mu(A, X, a) = 1, \quad (4)$$

(2) predictors with the same frequency of errors on train sample are indistinguishable,

$$n(a, X) = n(b, X) \longrightarrow \mu(A, X, a) = \mu(A, X, b), \quad (5)$$

(3) the training result is invariant with respect to replacing the set of predictors A by $\pi(A)$

$$\mu(A, X, a) = \mu(\pi A, \pi X, \pi a). \quad (6)$$

The first condition implies "probabilistic" normalization of weights of the predictors and ensures the zero "probabilities" to the predictors that do not belong to the set A. The second condition means that for any decomposition $\mathbb{X} = X \sqcup \bar{X}$, $X \in [\mathbb{X}]^l$, the probability to obtain the predictor as a result of training depends only on the number of algorithm's errors on train sample. The third condition means that the training result is not affected if the permutation π acts upon the set of objects $[\mathbb{X}]^l$ and on the set of predictors $\mathbb{A}$ simultaneously.

The following mapping is a constructive example of the randomized learning algorithm, which we call a *randomized method of empirical risk minimization*

$$\mu(A, X, a) = \frac{[a \in A(X)]}{|A(X)|}. \quad (7)$$

Theorem 1. *Mapping* (7) *is a randomized learning algorithm.*

Proof. We can check the first condition explicitly

$$\sum_{a \in A} \mu(A, X, a) = \sum_{a \in A(X)} \frac{1}{|A(X)|} = 1.$$

To prove the second proposition, it is sufficient to note that two predictors a_1 and a_2 with the same number of errors in the course of training can belong to the set $A(X)$ only simultaneously. Hence, the probability to obtain each of the predictors as a result of training is either zero or $\frac{1}{|A(X)|}$.

To prove the third condition, it is sufficient to prove that

$$a_0 \in \operatorname*{Argmin}_{a \in A} n(a, X) \Leftrightarrow \pi a_0 \in \operatorname*{Argmin}_{a \in \pi A} n(a, \pi X).$$

Using Lemma 1.1, we make the following chain of equivalent statements

$$\begin{aligned} a_0 \in \operatorname*{Argmin}_{a \in A} n(a, X) &\Leftrightarrow \forall a \in A \longrightarrow n(a_0, X) \le n(a, X) \\ &\Leftrightarrow \forall a \in A \longrightarrow n(\pi a_0, \pi X) \le n(\pi a, \pi X) \\ &\Leftrightarrow \forall a' \in \pi A \longrightarrow n(\pi a_0, \pi X) \le n(a', \pi X) \\ &\Leftrightarrow \pi a_0 \in \operatorname*{Argmin}_{a \in A} n(a, \pi X). \end{aligned}$$

The theorem is proved.

1.3. Overfitting Probability

The variable $\nu(a, U) = n(a, U)/|U|$ is called *the frequency of errors* of the predictor a on the sample U. We define the *deviation of frequencies* on the decomposition $\mathbb{X} = X \sqcup \bar{X}$ as the difference between the frequencies for the test and training samples: $\delta(a, X) = \nu(a, \bar{X}) - n(a, X)$.

We fix the parameter $\varepsilon \in (0, 1]$. We say that the predictor *a is overtrained* for the decomposition $X \sqcup \bar{X}$ if $\delta(a, X) \ge \varepsilon$.

We make the main (and the only) probabilistic assumption that all decompositions of the general sample into observable and hidden subsamples are equiprobable [3, 4].

If $\varphi: [\mathbb{X}]^l \longrightarrow \{\text{true, false}\}$ is a predicate, we call *the probability of the event* $\varphi(X)$ the fraction of decompositions of the sample such that the predicate $\varphi(X)$ is true

$$\mathbf{P}[\varphi(X)] = \frac{1}{C_L^l} \sum_{X \in [\mathbb{X}]^l} [\varphi(X)].$$

Hence, the mathematical expectation of the arbitrary function $x: [\mathbb{X}]^l \longrightarrow \mathbb{R}$ is

$$\mathbf{E}\xi(X) = \frac{1}{C_L^l} \sum_{X \in [\mathbb{X}]^l} \xi(X).$$

We call the variable

$$P_\mu(a, A) = \mathbf{E}\mu(A, X, a) \quad (8)$$

the probability to obtain the predictor $a \in A$ as a result of training.

For an arbitrary $\varepsilon \in (0, 1]$, we give the *contribution* the predictor $a \in A$ makes into the overfitting probability

$$Q_\mu(\varepsilon, a, A) = \mathbf{E}\mu(A, X, a)[\delta(a, X) \ge \varepsilon]. \quad (9)$$

We define the *overfitting probability* as the sum of contributions over all predictors

$$\begin{aligned} Q_\mu(\varepsilon, A) &= \sum_{a \in A} Q_\mu(\varepsilon, a, A) \\ &= \mathbf{E} \sum_{a \in A} \mu(A, X, a)[\delta(a, X) \ge \varepsilon]. \end{aligned} \quad (10)$$

We can simplify this definition for the deterministic learning algorithm $\mu: 2^{\mathbb{A}} \times [\mathbb{X}]^l \longrightarrow \mathbb{A}$

$$\begin{aligned} Q_\mu 9(\varepsilon, A) &= \mathbf{E} \sum_{a \in A} [\mu(A, X) = a][\delta(a, X) \ge \varepsilon] \\ &= \mathbf{E}[\delta(\mu(A, X), X) \ge \varepsilon]. \end{aligned}$$

The obtained expression is literally "the fraction of decompositions of the sample into the learning and test samples such that the chosen predictor $a = \mu(A, X)$ is overtrained."

Definition 2. ERM algorithms $\mu_o X = \arg\min_{a \in A(X)} n(a, \bar{X})$,

$$\mu_p X = \arg\max_{a \in A(X)} n(a, \bar{X})$$

are called *optimistic* and *pessimistic*, respectively.

Theorem 2. *Let μ be the randomized method of empirical risk minimization. For an arbitrary set of predictors $A \subseteq \mathbb{A}$ and each $\varepsilon \in (0, 1]$, the inequalities hold*

$$Q_{\mu_o}(\varepsilon, A) \le Q_\mu(\varepsilon, A) \le Q_{\mu_p}(\varepsilon, A). \quad (11)$$

This theorem lets us call the methods μ, μ_p, and μ_o, respectively, the choice of random, worst, and best predictors among the predictors best in the course of learning.

Proof. For the sake of brevity, we write the mappings μ_o and μ_p without the argument A. We show that the proposition holds for each decomposition of the sample

$$[\delta(\mu_o(X), X) \ge \varepsilon]$$

$$\le \sum_{a \in A(X)} \frac{1}{|A(X)|} [\delta(a, X) \ge \varepsilon] \le [\delta(\mu_p(X), X) \ge \varepsilon].$$

We introduce the designations

$$F_o \equiv [\delta(\mu_o(X), X) \ge \varepsilon],$$
$$F_p \equiv [\delta(\mu_p(X), X) \ge \varepsilon],$$

$$F \equiv \frac{1}{|A(X)|} \sum_{a \in A(X)} [\delta(a, X) \ge \varepsilon].$$

We consider the inequality $F_o \le F$. Note that F_o can take only two values, 0 and 1, and the value of the expression F is bounded by the segment [0, 1]. Hence, if $F_o = 0$, the inequality holds automatically.

We prove that $F_o = 1$ follows from $F = 1$. We denote $a_o \equiv \mu_o(X)$. By definition of μ, $a_o \in A(X)$ and $\forall a \in A(X)$ $n(a_o, \bar{X}) \le n(a, \bar{X})$. Hence, $\forall a \in A(X)$ $\delta(a, X) \ge \delta(a_o, X) \ge \varepsilon$. Thus, $F = \sum_{a \in A(X)} \frac{1}{|A(X)|} = 1$.

To prove $F \le F_p$, it is sufficient to consider two cases, $F_p = 0$ and $F_p = 1$, and perform similar reasoning.

2. SYMMETRY OF SETS OF PREDICTORS

With the concepts introduced above, we can define the group of symmetry of the set of predictors and use it to obtain computationally efficient formulas of the overfitting probability.

2.1. Invariance of the Overfitting Probability to the Action of the Group S_L

The definitions of the functionals $P_\mu(a, A)$, $Q_\mu(\varepsilon, a, A)$, and $Q_\mu(\varepsilon, A)$ relied on the fact that the objects of the general sample $\mathbb{X}$ are arranged. We prove that these functionals are invariant to the change of numeration of the objects in $\mathbb{X}$.

For the sake of brevity of designations, we omit the argument ε in the function $Q_\mu(\varepsilon, a, A)$.

Lemma 2. *The probability $P_\mu(a, A)$ of obtaining the predictor a as a result of training and the contribution $Q_\mu(a, A)$ the predictor a makes into the overfitting probability preserve for an arbitrary permutation $\pi \in S_L$ simultaneously applied to the set A and the predictor a*

$$P_\mu(a, A) = P_\mu(\pi a, \pi A), \quad (12)$$

$$Q_\mu(a, A) = Q_\mu(\pi a, \pi A). \quad (13)$$

Proof. Note that $\mathbf{E}f(X) = \mathbf{E}f(\pi X)$ holds for the arbitrary function $f(X)$ of the decomposition of the sample $X \sqcup \bar{X}$ into the learning and test samples. We also use the property $\delta(\pi a, \pi X) = \delta(a, X)$ that follows from Lemma 1 and the definition of deviation of frequencies of the predictor's errors. Then,

$$\begin{aligned} Q_\mu(\pi a, \pi A) &= \mathbf{E}\mu(\pi A, X, \pi a)\delta(\pi a, X) \ge \varepsilon \\ &= \mathbf{E}\mu(\pi A, \pi X, \pi a)[\delta(\pi a, \pi X) \ge \varepsilon] \\ &= \mathbf{E}\mu(A, X, a)[\delta(a, X) \ge \varepsilon] = Q_\mu(a, A). \end{aligned}$$

The equality $P_\mu(\pi a, \pi A) = P_\mu(a, A)$ is obtained from the expression $Q_\mu(a, A) = Q_\mu(\pi a, \pi A)$ by putting $\varepsilon = -1$.

Corollary 1. The overfitting probability preserves when an arbitrary permutation $\pi \in S_L$ is applied to the set of predictors

$$Q_\mu(A) = Q_\mu(\pi A). \quad (14)$$

Proof.

$$Q_\mu(\pi A) = \sum_{a \in \pi A} Q_\mu(a, \pi A)$$

$$= \sum_{a \in A} Q_\mu(\pi a, \pi A) = \sum_{a \in A} Q_\mu(a, A) = Q_\mu(A).$$

The latter proposition looks very natural since the order of objects in the sample does not matter in most problems of learning from precedents.

2.2. Group of Symmetry of the Set of Predictors

We recall that we defined the action of the group S_L on the set of all possible sets of predictors $2^{\mathbb{A}}$ above.

Definition 3. The stationary subgroup $\mathrm{Sym}(A)$ of the set of predictors $A \in 2^{\mathbb{A}}$ is called its *group of symmetry*

$$\mathrm{Sym}(A) = \{\pi \in S_L : \pi A = A\}.$$

Example. We consider the set of predictors given by the matrix of errors

$$\begin{array}{c} \\ x_1 \\ x_2 \\ x_3 \\ x_4 \\ x_5 \end{array} \begin{array}{c} \begin{array}{ccccc} a_1 & a_2 & a_3 & a_4 & a_5 \end{array} \\ \begin{pmatrix} 1 & 1 & 1 & 0 & 0 \\ 0 & 1 & 1 & 1 & 0 \\ 0 & 0 & 1 & 1 & 1 \\ 1 & 0 & 0 & 1 & 1 \\ 1 & 1 & 0 & 0 & 1 \end{pmatrix} \end{array}.$$

The rows of the matrix correspond to the objects of the general sample $\mathbb{X}$; the columns, to the predictors $a \in A$. The group of symmetry of this set is a dihedral group: $\mathrm{Sym}(A) \cong S_2 \ltimes \mathbb{Z}/5\mathbb{Z}$. The circular permutation $\pi_\circlearrowright = (x_1, x_2, x_3, x_4, x_5)$ and a pair of transpositions $\pi_\leftrightarrow = (x_2, x_5)(x_3, x_4)$ are the group-forming elements.

It is significant that the group of symmetry $\mathrm{Sym}(A)$ *acts* upon the set of predictors A. Indeed, each element of the group of symmetries $\pi \in \mathrm{Sym}(A)$ permutates the predictors a only *inside* the set A. Hence, for any $a \in A$ and any $\pi \in \mathrm{Sym}(A)$, $\pi a \in A$ holds. Therefore, for the group $\mathrm{Sym}(A)$, unlike the entire S_L, the action on the set A is given naturally.

The subset G is called the *orbit* of the element m of the set M, on which the group $Gm = \{gm: g \in G\} \subseteq M$ acts. Either the orbits of two elements m_1 and m_2 do not overlap or they coincide. This allows us to speak of the decomposition of the set M into the nonoverlapping orbits $M = Gm_1 \sqcup \ldots \sqcup Gm_k$.

In what follows, we consider the orbits of action of the group of symmetry $\mathrm{Sym}(A)$ on the set of predictors. We denote all the orbits of the set of predictors A by $\Omega(A)$. We denote the representative of the orbit $\omega \in \Omega(A)$ by $a_\omega \in A$.

Points of one orbit are called equivalent in group theory. Since, in [1], predictors with equal vectors of errors on the general sample $\mathbb{X}$ are also called *equivalent*, we call different representatives of the same orbit *identical predictors*.

Lemma 3. *Identical predictors have the same number of errors on the complete sample*.

The proof of the lemma automatically follows from Lemma 1

$$n(a, \mathbb{X}) = n(\pi a, \pi X) = n(\pi a, X).$$

By the definition given above, the predictor $a \equiv (a(x_i))_{i=1}^L$ is the vector, and, hence, it depends on the numeration of the objects of the sample. However, neither the group of symmetries $\mathrm{Sym}(A)$ nor the decomposition into classes of identical predictors $\Omega(A)$ depend on this numeration.

Lemma 4. *For any set of predictors $A \in 2^{\mathbb{A}}$ and any permutation $\pi \in S_L$, the groups* $\mathrm{Sym}(A)$ *and* $\mathrm{Sym}(\pi A)$ *are conjugate*: $\mathrm{Sym}(\pi A) = \pi \circ \mathrm{Sym}(A) \circ \pi^{-1}$.

This lemma is equivalent to the known proposition of the group theory; i.e., the stationary subgroups of points belonging to one orbit can be obtained from each other by conjugation [7].

Lemma 5. *Let the predictors a_1 and a_2 be identical in the set of predictors A. Then, $\forall \pi \in S_L$ the predictors πa_1 and πa_2 are identical in the set of predictors πA.*

Let $\gamma \in \mathrm{Sym}(A)$ be the permutation such that $a2 = \gamma a_1$. Then, $\pi a_2 = \pi\gamma a_1 = (\pi\gamma\pi^{-1})\pi a_1 = \tilde{\gamma}\,\pi a_1$. We have from Lemma 4 that $\tilde{\gamma} = \pi\gamma\pi^{-1}$ is the element of $\mathrm{Sym}(\pi A)$.

2.3. Theorems on the Equal Contribution of Identical Predictors into the Overfitting Probability

The theorems we give in this section can be useful for obtaining explicit formulas for the overfitting probability.

Theorem 3. Identical predictors have the same probability to be implemented as a result of training and make the same contribution to the overfitting probability

$$P_\mu(a, A) = P_\mu(\pi a, A), \tag{15}$$

$$Q_\mu(a, A) = Q_\mu(\pi a, A), \tag{16}$$

where $\pi \in \mathrm{Sym}(A)$.

The proof automatically follows from Lemma 2 and the definition of the group of symmetry $P_\mu(\pi a, A) = P_\mu(\pi a, \pi A) = P_\mu(a, A)$, and similarly for $Q_\mu(a, A)$.

Corollary 2. Let the group of symmetry act on the set of predictors transitively $A = \{\pi a_0, \pi \in \mathrm{Sym}(A)\}$, where $a_0 \in A$ is the arbitrary predictor of the set A. Then, all predictors of the set have the same probability to be implemented as a result of training.

Theorem 3 allows us to move from summing over all predictors of the set to summing over the orbits of the group $\mathrm{Sym}(A)$.

Theorem 4. *We can write the overfitting probability $Q_\mu(A)$ for the randomized method of empirical risk minimization as*

$$Q_\mu(A) = \sum_{\omega \in \Omega(A)} |\omega| \mathbf{E} \frac{[a_\omega \in A(X)]}{|A(X)|} [\delta(a_\omega, X) \geq \varepsilon]. \tag{17}$$

We apply the theorem on the equivalent contribution identical predictors make into the overfitting probability followed by definitions (9) and (7)

$$Q_\mu(A) = \sum_{a \in A} Q_\mu(a, A) = \sum_{\omega \in \Omega(A)} |\omega| Q_\mu(a_\omega, A)$$

$$= \sum_{\omega \in \Omega(A)} |\omega| \mathbf{E} \frac{[a_\omega \in A(X)]}{|A(X)|} [\delta(a_\omega, X) \geq \varepsilon].$$

Formula (17) is the main tool to derive accurate estimates of the overfitting probability for the randomized method of empirical risk minimization.

3. ACCURATE ESTIMATES OF THE OVERFITTING PROBABILITY

In this section, we obtain explicit combinatorial formulas for the functional $Q_\mu(\varepsilon, A)$ for some sets of predictors A possessing the property of symmetry.

3.1. The Complete Layer of Predictors

The set consisting of all predictors $a \in \mathbb{A}$ with a fixed number of errors $n(a, \mathbb{X}) = m$ is called the *complete m-layer* of predictors.

Theorem 5. *For training by the empirical risk minimization method, the overfitting probability for the complete m-layer of predictors is*

$$Q_\mu(\varepsilon, A) = [\varepsilon k \le m \le L - \varepsilon l]. \quad (18)$$

Proof. In this case, the entire symmetric group S_L is the group of symmetry Sym(A). Hence, the action of the group of symmetry on the set of predictors is transitive, and the set has only one class of identical predictors from C_L^m. By theorem 4, we write

$$Q_\mu(\varepsilon, A) = C_L^m \mathbf{E} \frac{[a_0 \in A(X)]}{|A(X)|} [\delta(a_0, X) \ge \varepsilon],$$

where a_0 is an arbitrary predictor of the set.

The predictor a_0 will be chosen only if it makes a minimal number of errors in the course of training. We consider two cases.

Case 1. $m \le k$. All errors of a_0 go to the test sample, with overfitting happening if $m \ge \varepsilon k$. This fixes m objects of the test sample. Hence, the number of summands in the sum over decompositions X is the number of ways to choose $k - m$ objects such that the predictor a_0 does not make any error. This number is C_{L-m}^{k-m}.

The cardinality of the set of the predictors $A(X)$ best in training is independent of X and is C_k^m, i.e., the number of ways to place m errors of the predictors in k positions of the test sample. Thus,

$$Q_\mu(\varepsilon, A) = \frac{C_L^m}{C_L^l} \frac{C_{l-m}^{k-m}}{C_k^m} [m \ge \varepsilon k] \quad \text{for} \quad m \le k.$$

Case 2. $m > k$. The test sample must consist only of objects on which a_0 makes errors. Then, there are $m - k$ errors left in the training process, and the overfitting condition is $1 - \frac{m-k}{l} \ge \varepsilon$. Hence, $m \le L - \varepsilon l$.

The number of decompositions of the sample, for which $a_0 \in A(X)$, is C_m^k, i.e., the number of ways to choose k errors of the predictor a_0 for the test sample. The cardinality of the set $A(X)$ again does not depend on X and is C_l^{m-k}, i.e., the number of ways to choose $m - k$ errors for the learning sample

$$Q_\mu(\varepsilon, A) = \frac{C_L^m}{C_L^l} \frac{C_l^{m-k}}{C_m^k} [m \le L - \varepsilon l] \quad \text{for} \quad m > k.$$

Writing the identity $C_L^k = \frac{L!}{k!(L-k)!}$ for each combinatorial coefficient, we find that the combinatorial factors are unity in both formulas. Combining the conditions $\varepsilon k \ge m \ge k$ and $k < m \le L = \varepsilon l$, we obtain the theorem's hypothesis.

3.2. Cube of Predictors

We call the cube of predictors $\mathbb{A}$ the set that includes all possible Boolean vectors $a \in \{0, 1\}^L$.

Theorem 6. *The overfitting probability for the cube of predictors is given by the formula*

$$Q_\mu(\varepsilon, \mathbb{A}) = \frac{1}{2^k} \sum_{m = \lceil \varepsilon k \rceil}^{k} C_k^m.$$

Proof. Obviously, in this case, the group of symmetry is the entire S_L. Then, the layers of predictors with the same number of errors are its orbits. Therefore, by Theorem 4,

$$Q_\mu(\varepsilon, \mathbb{A}) = \sum_{m=0}^{L} C_L^m \mathbf{E} \frac{[a_m \in A(X)]}{|A(X)|} [\delta(a, X) \ge \varepsilon].$$

The predictor can be chosen as a result of training only if it makes no errors in the course of training. Therefore, all its errors should go to the test sample. Hence, we can limit the summation index to $m \le k$.

Since all errors of the chosen predictor are in the test sample, the deviation of the frequencies is $\delta(a, X) = \frac{m}{k}$ for any decomposition. Hence, the overfitting happens for $m \ge \lceil \varepsilon k \rceil$.

There are always 2^k predictors in the set $A(X)$. The predictors have zero errors in the course of training and all possible vectors of errors on the test sample.

Combining all the established facts, we obtain the formula

$$Q_\mu(\varepsilon, \mathbb{A}) = \sum_{m = \lceil \varepsilon k \rceil}^{k} C_L^m \frac{\mathbf{E}[a_m \in A(X)]}{2^k}.$$

Now, we have to calculate the number of decompositions on which the predictor a_m is chosen by the learning algorithm. This is the number of ways to choose l objects of the learning sample from L correct answers of the predictor a_m. Finally, we have

$$Q_\mu(\varepsilon, \mathbb{A}) = \sum_{m = \lceil \varepsilon k \rceil}^{k} C_L^m \frac{C_{L-m}^l}{C_L^l 2^k} = \frac{1}{2^k} \sum_{m = \lceil \varepsilon k \rceil}^{k} C_k^m.$$

3.3. Unimodal Chain

We find the distance between predictors $\rho(a, a')$ as the Hamming distance between their vectors of errors

$$\rho(a, a') = \sum_{x \in X} |a(x) - a'(x)|.$$

Definition 4. The set of predictors $\{a_0, ..., a_D\}$ is called a *monotonic chain* if two conditions are met:

(1) the number of errors is monotonic: $n(a_i, \mathbb{X}) = m + i$, $i = 0, ..., D$ for some fixed m,

(2) errors of the previous predictor are absorbed: $\rho(a_i, a_{i-1})$, $i = 1, ..., D$.

Thus, every subsequent predictor in the monotonic chain makes errors on the same objects as the previous predictor and one additional error.

The monotonic chain of predictors is the simplest model of a one-parametric *connected set of predictors* implying that the number of errors on the complete sample increases as some parameter continuously moves away from its optimal value.

Definition 5. The set of predictors $\{a_0, a_1, ..., a_D, a'_1, ..., a'_D\}$ is called a unimodal chain if two conditions are met:

(1) its left $\{a_0, a_1, ..., a_D\}$ and right $\{a_0, a'_1, ..., a'_D\}$ branches are monotonic chains,

(2) the overlapping of the set of errors of predictors a_D and a'_D is the set of errors of the predictor a_0.

The unimodal chain is a more realistic model of the one-parametric *connected set* as compared to the monotonic chain. If we have the best predictor a_0 with the optimal value of some real parameter, the deviation of the value of this parameter both upward and downward makes the number of errors increase.

Theorem 7. *For the unimodal chain with branches of length D, the overfitting probability of the randomized method of empirical risk minimization is*

$$Q_\mu(\varepsilon, A) = \sum_{h=0}^{D} \sum_{t_1=h}^{D} \sum_{t_2=0}^{D} \frac{|\omega_h|}{1 + t_1 + t_2} \frac{C_{L'}^{l'}}{C_L^l} H_{L'}^{l', m}(s(\varepsilon)), \quad (19)$$

where $L' = L - t_1 - t_2 - F$, $F = [t_1 \neq D] + [t_2 \neq D]$, $l' = l - F$, $s(\varepsilon) = \left\lfloor \frac{l}{L}(m + h - \varepsilon k) \right\rfloor$, $|\omega_h| = 1$ for $h = 0$ and $|\omega_h| = 2$ for $h \geq 1$; $H_{L'}^{l', m}(z) = \frac{1}{C_{L'}^{l'}} \sum_{s=0}^{\lfloor z \rfloor} C_m^s C_{L'-m}^{l'-s}$ is the function of hypergeometric distribution [4].

Proof. We numerate the objects of the general sample $\mathbb{X}$ as shown in the table

	a_0	a_1	a_2	...	a_D	a'_1	a'_2	...	a'_D
x_1	0	1	1	...	1	0	0	...	0
x_2	0	0	1	...	1	0	0	...	0
...	...	...	...	...	...	...	...	...	...
x_D	0	0	0	...	1	0	0	...	0
x'_1	0	0	0	...	0	1	1	...	1
x'_2	0	0	0	...	0	0	1	...	1
...	...	...	...	...	...	...	...	...	...
x'_D	0	0	0	...	0	0	0	...	1

Permutating the objects of the sample ($x_1 \longleftrightarrow x'_1, ..., x_D \longleftrightarrow x'_D$), we can rearrange the left and right branches. Therefore, identical in the unimodal chain are the pairs of predictors with the same number of errors on the complete sample.

By Theorem 4, we can write the overfitting probability as

$$Q_\mu(\varepsilon, A) = \sum_{h=0}^{D} |\omega_h| \sum_{t_1=h}^{D} \sum_{t_2=0}^{D} \frac{1}{C_L^l} \times \sum_{X \in N(t_1, t_2)} \frac{1}{|A(X)|} [\delta(a_h, X) \geq \varepsilon].$$

Here, the index h denotes the number of the class of identical predictors (so that all predictors of the class ω_h have $m + h$ errors); $|\omega_0| = 1$, and $|\omega_h| = 2$ for $h \geq 1$. For the sake of definiteness, we take the representative a_h of the class ω_h from the left branch of the chain.

The indices t_1 and t_2 parameterize the content of the set $A(X)$. For an arbitrary decomposition $X \in [\mathbb{X}]^l$, we give t_1 as the maximal number for which all objects $x_1, x_2, ..., x_t$ are in the test sample and x_{t_1+1}, if it exists, is in the learning sample. The index t_2 is given similarly for the objects of the right branch. The set $N(t_1, t_2) \subset [\mathbb{X}]^l$ is the set of all decompositions with the parameters t_1 and t_2.

It follows from the definition of t_1 and t_2 that $|A(X)| = \frac{1}{1 + t_1 + t_2}$. Within the summation, the indices t_1 and t_2 take various sets of values since we consider only those decompositions for which the representative a_h chosen from the left branch lies in $A(X)$.

We denote $F = [t_1 \neq D] + [t_2 \neq D]$, $L' = L - t_1 - t_2 - F$, $l' = l - F$. The parameter F allows us to take into account the contribution of the last predictors a_D and a'_D of the chain.

We calculate the cardinality of the subset of those decompositions from $N(t_1, t_2)$ on which the predictor a_h is overtrained. Let $s_0(\varepsilon)$ be the maximal number of errors in the course of training for which we have overfitting. By the definition of deviation of frequencies, we find $s_0(\varepsilon) = \left\lfloor \frac{l}{L}(m + h - \varepsilon k) \right\rfloor$. We need to choose l' objects from L' for training so that there are no more than $s_0(\varepsilon)$ errors of m free errors of the predictor a_h in the training. The number of ways is $\sum_{s=0}^{s_0(\varepsilon)} C_m^s C_{L'-m}^{l'-s}$.

Combining all results, we obtain the final formula

$$Q_\mu(\varepsilon, A) = \sum_{h=0}^{D} |\omega_h| \sum_{t_1=h}^{D} \sum_{t_2=0}^{D} \frac{1}{1 + t_1 + t_2} \frac{C_{L'}^{l'}}{C_L^l} H_{L'}^{l', m}(s_0(\varepsilon)).$$

3.4. Bundle of Monotonic Chains

A bundle of p monotonic chains is the set of predictors obtained by combining p monotonic chains of the same length with the common first predictor. As for the unimodal chain, we assume that the sets of objects on which the predictor makes errors do not overlap.

The group of symmetry of the bundle of p monotonic chains is the symmetrical group S_p that acts upon the branches of the bundle by various permutations. Thus, the classes of identical predictors are the subsets of predictors with the same number of errors on the complete sample called *layers* [4].

The following theorem gives the explicit formula for the overfitting probability for the bundle of p monotonic chains. We introduce a *combinatorial coefficient* $R_{D,p}^h(S, F)$ that depends on the parameters S and F, on the number of monotonic chains p, and on their length D, as well as on h, which is the minimal value of the parameter S. The coefficient $R_{D,p}^h(S, F)$ is the number of ways to represent the value S as the sum of p nonnegative summands, $S = t_1 + \ldots + t_p$, each of which does not exceed D. F summands exactly should not equal D, with an additional restriction $t_1 \geq h$ imposed on the first summand.

Theorem 8. *Let the bundle of p monotonic chains have the best predictor making m errors on the complete sample, and the length of each branch is D, leaving the best predictor aside. Then, for training performed by the randomized method, we can write the overfitting probability as*

$$Q_\mu(\varepsilon, A) = \sum_{h=0}^{D} \sum_{S=h}^{pD} \sum_{F=0}^{p} \frac{|\omega_h| R_{D,p}^h(S, F)}{1 + S} \times \frac{C_{L'}^{l'}}{C_L^l} H_{L'}^{l', m}(s(\varepsilon)), \quad (20)$$

where $L' = L - S - F$, $l = l - F$, $s(\varepsilon) = \left\lfloor \frac{l}{L}(m + h - \varepsilon k) \right\rfloor$; $|\omega_h| = 1$ *for* $h = 0$ *and* $|\omega_h| = p$ *for* $h \geq 1$; $H_{L'}^{l', m}(s)$ *is the function of hypergeometric distribution* [4].

Proof. Generalizing the reasoning given for the unimodal chain in a natural way, we obtain the formula

$$Q_\mu(\varepsilon, A) = \sum_{h=0}^{D} |\omega_h| \times \sum_{t_1=h}^{D} \sum_{t_2=0}^{D} \cdots \sum_{t_p=0}^{D} \frac{1}{1 + t_1 + t_2 + \ldots + t_p} \frac{C_{L'}^{l'}}{C_L^l} H_{L'}^{l', m}(s(\varepsilon)),$$

where $L' = \mathrm{L} - \sum_{i=1}^{p} t_i - \sum_{i=1}^{p} [t_i \neq D]$, $l' = l - \sum_{i=1}^{p} [t_i \neq D]$, $s_0(\varepsilon) = \left\lfloor \frac{l}{L}(m + h - \varepsilon k) \right\rfloor$.

We use the additional designation $S = \sum_{i=1}^{p} t_i$, $F = \sum_{i=1}^{p} [t_i \neq D]$ to simplify the writing. The parameter S gives the cardinality of the set $A(X)$.

$$Q_\mu(\varepsilon, A) = \sum_{h=0}^{D} |\omega_h| \times \sum_{t_1=h}^{D} \sum_{t_2=0}^{D} \cdots \sum_{t_p=0}^{D} \frac{1}{1 + S} \frac{C_{L'}^{l'}}{C_L^l} H_{L'}^{l', m}(s_0(\varepsilon)),$$

where $L' = L - S - F$, $l' = l - F$, $s_0(\varepsilon) = \left\lfloor \frac{l}{L}(m + h - \varepsilon k) \right\rfloor$.

Now, we can pass from summing over the parameters t_i to summing over the set of all possible values S and F

$$Q_\mu(\varepsilon, A) = \sum_{h=0}^{D} |\omega_h| \sum_{S=h}^{pD} \sum_{F=0}^{p} \frac{R_{D,p}^h(S, F)}{1 + S} \frac{C_{L'}^{l'}}{C_L^l} H_{L'}^{l', m}(s_0(\varepsilon)),$$

where $R_{D,p}^h(S, F)$ is the combinatorial coefficient defined above.

The bundle of $2p$ monotonic chains is a model of the p-parametric set of predictors, in which one can change any of p parameters for other parameters fixed and cannot change several parameters at a time. This set can be treated as the generalization of three special cases considered in [3], i.e., the monotonic chain ($p = 1$), the unimodal chain ($p = 2$), and the unit neighborhood of the best predictor ($D = 1$).

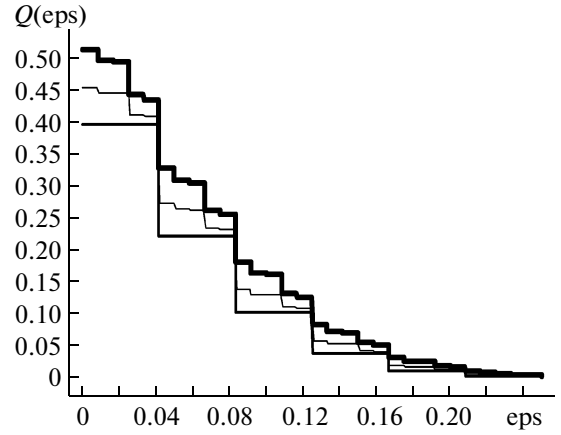

Fig. 1. $Q_\mu(\varepsilon, A)$ depending on ε for the monotonic chain for $L = 100$, $l = 60$, $D = 40$, $m = 20$.

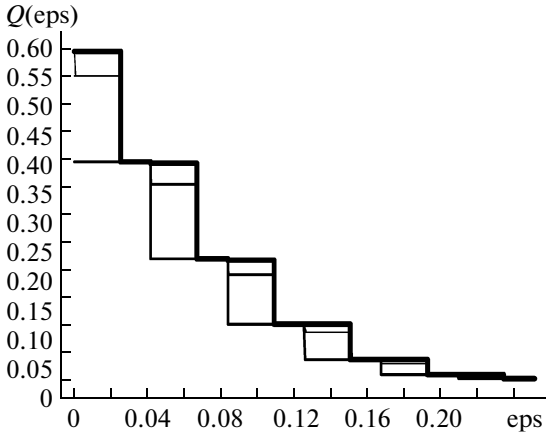

Fig. 2. $Q_\mu(\varepsilon, A)$ depending on ε for the unit neighborhood for $L = 100$, $l = 60$, $p = 10$, $m = 20$.

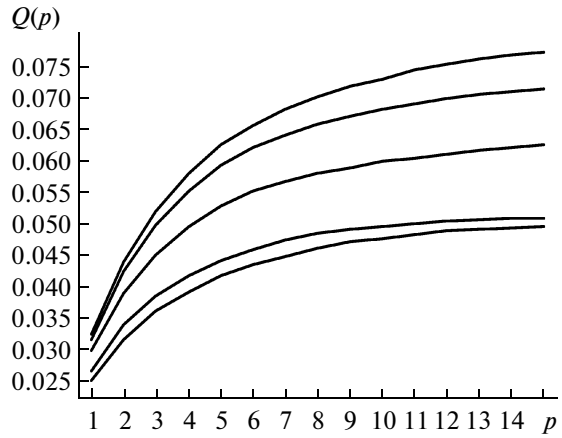

Fig. 3. $Q_\mu(\varepsilon, A)$ depending on p for the bundle of monotonic chains for $L = 300$, $l = 150$, $D = 1, 2, 3, 5, 10$, $\varepsilon = 0.05$.

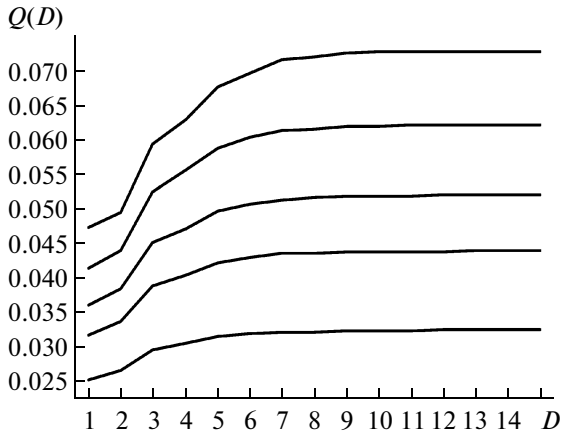

Fig. 4. $Q_\mu(\varepsilon, A)$ depending on D for the bundle of $p = 1, 2, 3, 5, 10$ monotonic chains for $L = 300$, $l = 150$, $m = 15$, $\varepsilon = 0.05$.

The formula for the overfitting probability for the unimodal chain was obtained in Theorem 7. To obtain explicit formulas for the two other families, it is sufficient to find the explicit expression for the combinatorial coefficient $R^h_{D,p}(S, F)$.

Corollary 3. For the monotonic chain of length $D + 1$, the overfitting probability is

$$Q_\mu(\varepsilon, A) = \frac{1}{C^l_L}\sum_{h=0}^{D}\sum_{S=h}^{D}\frac{1}{1+S}H^{l',m}_{L'}(s(\varepsilon)), \qquad (21)$$

where $L' = L - S - [S \neq D]$, $l' = l - [S \neq D]$.

Corollary 4. For the unit neighborhood of $p + 1$ predictors, the overfitting probability is

$$Q_\mu(\varepsilon, A) = \frac{1}{C^l_L}\sum_{h=0}^{D}\sum_{S=h}^{D}\frac{|\omega_h|C^{S-h}_{p-h}}{1+S}H^{l',m}_{L'}(s(\varepsilon)), \qquad (22)$$

where $L' = l - p$, $l' = l + S - p$.

3.5. Numerical Experiment

Figures 1 and 2 give the results of numerical experiments that compared overfitting probabilities for different options of empirical risk minimization. Each graph has four curves, with the upper (bold) one corresponding to pessimistic empirical risk minimization [3, 4] and the lower one, to optimistic empirical risk minimization. Two almost coinciding curves that lie between them stand for the randomized empirical risk minimization. One of them is calculated using the proved formulas, and the second one is constructed by the Monte Carlo method using 10^5 random decompositions, given the equiprobable choice of the best predictor in the case of uncertainty. The differences of these two curves lie within the error of the Monte Carlo method.

Figures 3 and 4 give the overfitting probability depending on the number of branches p in the bundle and their length D. The graphs are drawn for the ran-

domized empirical risk minimization method. Figure 4 shows that when the length of chains D increases, the overfitting probability almost stops growing as early as for $D = 7$. This is due to the *localization effect* [4], i.e., only predictors from lower layers have a substantially nonzero probability to be chosen by the empirical risk minimization method. Adding predictors that are "too bad" does not increase the overfitting probability. Figure 3 shows that the overfitting probability continues growing as the number of chains p in the bundle grows. However, the *connectivity effect* makes the growth rate sublinear with respect to p; i.e., all predictors are at a Hamming distance not greater than D from the best predictor.

4. CONCLUSIONS

With the symmetry property of families of predictors, we can obtain computationally efficient formulas for the overfitting probability. For the monotonic chain, the unimodal chain, and the unit neighborhood, we obtained formulas such as the corollary of one theorem, while similar estimates used to be proved independently and under a nonnatural assumption regarding a priori arrangement of predictors in the set [3]. The proposed approach allows obtaining estimates for the set with an exponentially growing number of predictors (the complete cube, the Boolean cube).

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REFERENCES

1. V. N. Vapnik and A. Ya. Chervonenko, *Pattern Recognition Theory* (Moscow, Nauka, 1974) [in Russian].
2. V. Vapnik, *Statistical Learning Theory* (New York, Wiley, 1998).
3. K. V. Vorontsov, "Accurate Estimates of Overtraining Probability," Doklady RAN, **429** (1), 15–18 (2009).
4. K. V. Vorontsov, "Combinatorial Approach to Overtraining," All-Russian Conference on Mathematical Methods of Pattern Recognition-14 (Moscow, MAKS Press, 2009), pp. 18–21.
5. P. V. Botov, "Accurate Estimates of Overtraining Probability for Monotonic and Unimodal Families of Algorithms," All-Russian Conference on Mathematical Methods of Pattern Recognition-14 (Moscow, MAKS Press, 2009), pp. 7–10.
6. A. I. Frei, "Accurate Estimates of Overtraining Probability for Symmetric Families of Algorithms," All-Russian Conference on Mathematical Methods of Pattern Recognition-14 (Moscow, MAKS Press, 2009), pp. 66–69.
7. E. B. Vinberg, *Algebra* (Moscow, Factorial Press, 2001) [in Russian].

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